Numerical research of capabilities of flat thermochemical reactor as element of a hypersonic flight vehicle heat protection

V.K. Vasilyev[*], A.V. Korabelnikov, A.V. Fedotov[**]

Introduction

Thermal protection of heat-stressed surfaces of a hypersonic flight vehicle (HFV), flying in dense layers of atmosphere with hypersonic velocities ($M \geq 7$), is now one of the most actual problems [1, 2]. In HFV developed under the "Ajax" concept it is supposed that in the most heat-stressed parts of a skin and engine the chemical catalytic reactors will be placed in which the high endothermic processes of decomposition of initial hydrocarbon fuel with the help of steam and carbon dioxide reforming of methane and its liquid homologues have to be implemented [3].

Such organization of the process of thermochemical conversion of hydrocarbons onboard a flight vehicle (FV) will enable [4]:

- to increase a portion of useful usage of a FV power resource at the expense of a chemical recuperation of heat losses connected as with aerodynamic heating of a skin under the hypersonic flight conditions and power plant operation;
- to increase cooling capability of fuel by means of physical-chemical transformations (heating, vaporization, endothermic reactions) of initial components;
- to provide an active thermal protection (ATP) of heat-stressed parts of construction using not only heat removal by means of convection and radiation, but also its absorption in a catalytic reaction run directly on the protected surface;
- to influence positively on the conditions of a FV airflow-around at the expense of a skin construction cooling;
- to obtain in reaction a synthesis gas (mixture of H_2 and CO) which will be directed to the combustion chamber for improvement of a fuel combustion characteristics.

Thermochemical reactors (TCR) of various kinds used as elements of a HFV thermal protection as usual should decide two problems:

1. To provide utilisation of heat fluxes with specific density from 50 kW / м^2 up to 1-2 MW/м^2 arising on the elements of HFV at moving in atmosphere with speeds at M = 7-15.

[*] - Russian Academy of Sciences, Moscow
[**] - Hypersonic Systems Research Institute, S.-Petersburg

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2. To create a fuel mixture with a defined chemical composition. For example, the volume concentration of H_2 in the obtained fuel mixture should not be less than 60 %.

As one of the elements of ATP a flat TCR can be used. It has a form of parallelepiped with length L, width l, height h ($h << L$, $h << l$) one of which walls is heated from outside, inside this wall is coated with catalyst, the second wall - is heat-insulated. At the TCR input the mixture of gaseous hydrocarbon C_nH_m and water vapour H_2O is supplied which components react on a catalytic wall.

The present numerical research is a first step in definition of TCR capabilities therefore the purposes of activity were the following:

- evaluation of heat flux utilised in the flat TCR;
- evaluation of a quantitative composition of a fuel mixture obtained at the TCR output.

Formulation of the task and computation method

In a flat TCR the ratio of its dimensions is: $h << L$, $h << l$, therefore it is possible to select a preferred direction of movement - lengthwise TCR (axis x). As the height of TCR is $h << l$, the flow in a flat TCR is mainly two-dimensional. Three-dimensionality will have an effect only near to corners of a parallelepiped but because of that $h << l$ its influence is very low. For such flows the approximation of a slender channel is applicable [5]. A system of differential partial equations defining a flow of viscous gas mixture with chemical reactions in approximation of a slender channel is a system of a parabolic type. For such system of equations the highly economical marching schemes are developed and used.

The numerous calculations have shown that application of a slender channel approach results at initial part of flow in an error not more than 10-15 % and at the distance of two or more gages it decreases up to 1-2 %.

As necessary condition for successful application of a system of slender channel equations is small local slope angles of channel walls to a centerline x, $|tg\theta| << 1$, or $|\theta| < 5^o$-7^o, the given approach can be applicable for calculation not only flat, but also slightly curved TCR.

The flow in TCR can be both laminar and turbulent. For uniformity of description of the both flow regimes the generally accepted «quasilaminar» approach was applied, according to which the heat and mass-exchange processes in turbulent flows are similar to the processes in laminar flows but with other proportionality ratios. This approach allows to introduce the concept of effective viscosity:

$$\mu_{eff} = \mu + \mu_T ,$$

where μ - factor of dynamic viscosity, μ_T - its turbulent analogue so that influence of turbulence is counted mainly with the help of the additive component to a viscosity coefficient.

At the first stage the factor of turbulent viscosity is determined by well-known Prandtle formula [6] in which in order to take into account interaction of molecular and molar transfers the damping Van-Drist factor was applied. After obtaining the experimental results and comparison them with calculating ones the updating of mathematical model as a whole and model of turbulence, in particular, is foreseen. Replacement of the Prandtle formula on more complicated model of turbulence, for example, on the two-parameter SST Mentor model or on the model of Reinolds' stresses is possible in the last case.

The system of equations describing the given flow is not presented here because of its awkwardness, however, this system is canonical and it is possible to acquaint with it in any monography on flow of viscous liquids, for example, [5,6].

Initial and the boundary conditions for a system of equations were set by a general mode: the conditions of adhesion were applied to components of velocity vector on a firm walls; for transversal speed the zero initial conditions were used, and the Puaseil parabola was applied to longitudinal speed at a laminar flow mode and the ratio $u \sim y^{1/7}$ at a turbulent flow mode [6]. The lower wall was considered as heat-insulated; on the upper wall for temperature T it is possible to use two types of boundary conditions: or first kind (T=Tw), or second kind $-\lambda \left.\frac{\partial T}{\partial y}\right|_w = Q_w$, where Q_w - specific heat flux [W / m^2].

Application of boundary conditions of the first kind from the mathematical point of view allows to define a heat flow Q (x) which is absorbed by the given specific gas mixture at the fixed input parameters. From the physical point of view usage of conditions of the first kind demonstrates what specific heat flux Q (x) it is necessary to set on the upper wall, that for the given gas mixture the temperature of heated surface remains constant.

Setting of boundary conditions of the second kind without the solution of conjugate problem on gas flow and heat conductivity in a solid body is physically incorrect as in a similar case apriori it is considered that gas can absorb the given heat flux. However, the given boundary conditions allow to evaluate a level of arising maximum temperatures in a solid body for different on intensity heat fluxes in combination with different parameters determining flow of gas mixture.

The gas mixture going into TCR was considered as uniformly mixed and uniformly heated, therefore, the temperature of a mixture T_{in} and concentrations of initial components at TCR input were considered constant along the height of reactor.

As a hydrocarbon the methane CH_4 was selected and the following chemical reactions were taken into account:

$$CH_4 + H_2O \leftrightarrow 3H_2O + CO ,$$

$$CO + H_2O \leftrightarrow H_2 + CO_2 ,$$

which were run only on a surface of catalytic wall. As it was marked in [5] three cases of chemical interaction are possible: $t_{ch} >> t_f$, $t_{ch} << t_f$, $t_{ch} \approx t_f$, here t_{ch} – typical time of a chemical reaction, t_f - typical time for gas mixture flow. The fist case corresponds to absence of chemical reactions, second, so-called equilibrium flow, corresponds to an indefinitely high speed of chemical reactions, third - to final velocity of chemical reactions.

At the present calculations the second case of chemical interaction with setting of boundary conditions of a first kind was studied. Study of equilibrium flows allows to evaluate the upper bound value of the utilised heat flow, concentrations of hydrogen H_2 and carbon monoxide CO. The first case (absence of chemical reactions, not catalytic wall) was calculated additionally for an estimation of influencing of chemical reactions on activity TCR. System of equations of a slender channel was solved by a finite-difference method [7], which was generalized for the case of compressed flows. As the system of equations describing the flow of gas mixture in flat TCR is essentially non-linear it was solved by the method of subsequent approximations. For improvement of iterations convergence and, therefore, decreasing of computer operating time the initial system of equations was divided into two subsystems: «dynamic» and «thermodynamic» which were solved independently up to full convergence of iterations in each subsystem, and the general solution was obtained at implementation of global iterations. At usage one or multiparameter model of turbulence the third subsystem, «turbulent», should be arisen which can be solved independently of two others or can be solved together with one of subsystems, as usual, «dynamic» one. The specific recommendations for solution of the «turbulent» subsystem can be given more often only after analysis of actual iterative process made on the computer.

Results of calculations

Heat fluxes

For a heat fluxes absorbed in TCR it is possible to write the following ratio:

$$Q = Q_f + Q_{chem},$$

where Q - heat flux absorbed in TCR, Q_f - heat flux absorbed by gas in the absence of chemical reactions, Q_{chem} - heat flow additionally absorbed in TCR at the expense of chemical reactions (for non-catalytic wall Q = Qf). For Qchem it is possible to write the following equality:

$$Q_{chem} = Q_{xp} + Q_d + Q_t, \quad (3)$$

where Q_{xp} - heat flux absorbed directly at the expense of reaction heat; Q_d - heat flow absorbed at the expense of change of the thermodynamic characteristics of a gas mixture, first of all, change of c_p due to chemical reactions; Qt - heat flux absorbed directly by gas (the same as Q_f) because at the presence of endothermic chemical reactions the temperature of mixture in TCR is less than without chemical reactions.

The analysis of the results of calculations has shown that $Q_t \approx 0$. It is explained by the fact that the change of mean temperature of mixture lengthwise of channel for catalytic and non-catalytic walls practically the same (fig. 1). $Q_d \approx 0.1Q_{chem}$, $Q_{xp} \approx 0.9Q_{chem}$. The preliminary calculations have shown that contribution of chemical reactions to heat removal in TCR can make approximately from 10 up to 70 % of total heat removal in TCR depending on a flow mode (laminar or turbulent) and input parameters of mixture. Optimization of TCR on the following parameters: total absorbed heat flux, efficiency of chemical reactions, composition of a mixture at TCR output - for each specific case is possible after a careful study of a specific TCR.

Results of calculations for TCR of height h = 4 mm are given below. At TCR input gas mixture has the following parameters: T_{in} = 400C, P=0,1Mpa, U_{in}=10m/s (G=0,012 kg/s), C_{CH4} = 0,5, C_{H2O}=0,5. Two flow modes - laminar and turbulent for two values of temperature of a heated catalytic wall were studied: T_w = 700 C and T_w = 1000 C.

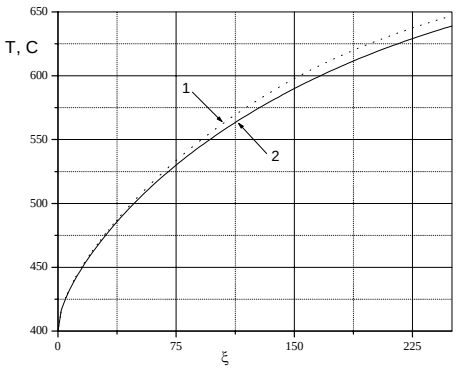

Fig. 1. Change of mean temperature of mixture lengthwise TCR, T_{in} = 400C: 1 - catalytic wall, 2 – non-catalytic wall.

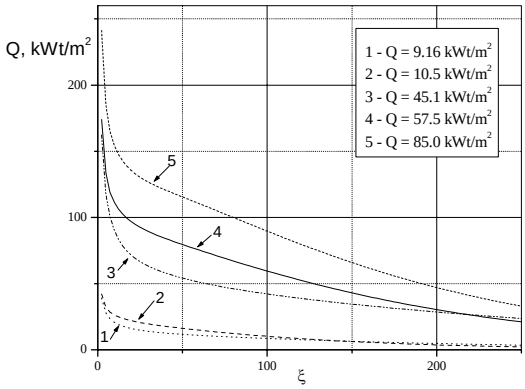

Fig. 2. Relationship of absorbed heat flux Q lengthwise TCR: 1 - T_w = 700 C, non-catalytic wall, laminar mode; 2 - T_w = 700 C, non-catalytic wall, turbulent mode; 3 - T_w = 700 C, catalytic wall, laminar mode; 4 - T_w = 700 C, catalytic wall, turbulent mode; 5 - T_w = 1000 C, catalytic wall, turbulent mode.

In fig. 2 for the different flow modes the relationship of absorbed heat flux on dimensionless coordinate $\zeta = x/h$ is shown and for these modes the values of mean absorbed specific heat fluxs are indicated. For all flow modes it is possible to distinguish two parts: initial $\zeta \leq 10$ and main one. At the initial part a sharp decreasing of absorbed heat flux is realised. It is explained by the fact that at this part the gas close to catalytic wall is rather cold and because of big temperature gradient in the near-wall area the heat absorption occurs first of all at the expense of the processes of molecular (laminar mode) or molar (turbulent mode) diffusion. At the main part a considerable role in heat absorption the chemical processes start to play.

At a turbulent flow mode the more intensive mixing of a gas transverse of TCR is realized, therefore at turbulent flow there is a more effective cooling than in laminar flow. The curves of absorption of heat flux 1 and 2 (turbulent and laminar chemically non-reactive flow modes) and 3 and 4 (turbulent and laminar chemically reacting flow modes) are intersected - 1 and 2 at $\zeta \approx 150$, 3 and 4 at $\zeta \approx 225$. It is explained by the fact that turbulence provides the intensive input of more cold and chemically non-reacted gas to a catalytic wall and therefore the gas mixture more quickly «exhausts its capabilities» of heat absorption. However, mean temperature of a mixture at turbulent flow at the distance of 250 gages from a channel input remains less than at a corresponding laminar mode. Comparing the laminar and turbulent flow modes it is possible to draw a conclusion that the turbulent mode provides more intensive cooling. However, probably, at cooling of extended weakly heat-stressed surfaces a laminar flow mode will be more expedient, than turbulent one.

Chemical composition of mixture

In fig. 3-7 the change of mean mole concentration of CH_4, H_2O, H_2, CO, CO_2 for three flow modes with catalytic wall is shown: laminar T_w = 700 C, turbulent T_w = 700C and turbulent T_w = 1000C. In these figures: curve 1 - laminar mode, T_w = 700C, curve 2 - turbulent mode, T_w = 700C, curve 3 - turbulent mode, T_w = 1000C. It is possible to mark that in spite of the fact that the turbulent flow mode provides higher concentration of molecular hydrogen than laminar one, the difference in mole concentration of H_2 depending on a flow mode is insignificant - for T_w = 700C $C_{H2} \approx 0.5$ for laminar flow, and $C_{H2} \approx 0.58$ for turbulent flow. In a fig. 8 the change of mole composition of mixture lengthwise TCR for turbulent flow with catalytic wall and T_w = 1000 C is shown.

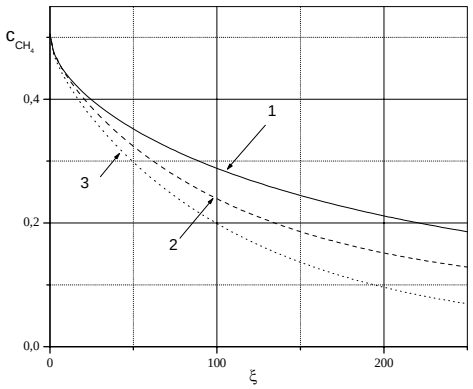

Fig. 3. Mole concentration of CH_4 lengthwise TCR

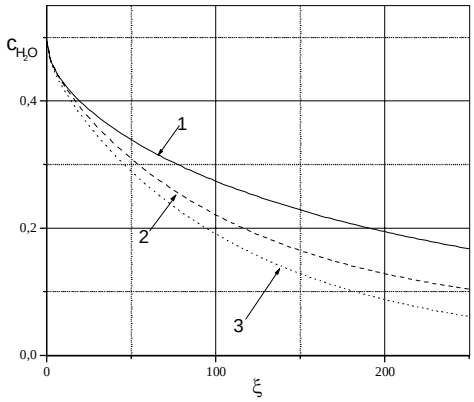

Fig. 4. Mole concentration of H_2O lengthwise TCR

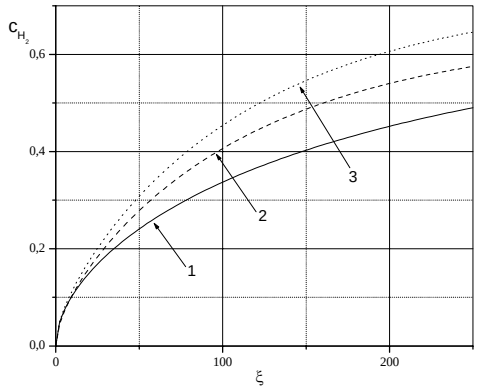

Fig. 5. Mole concentration of H_2 lengthwise TCR

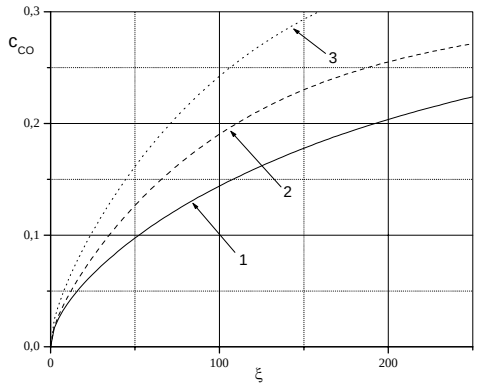

Fig. 6. Mole concentration of CO lengthwise TCR

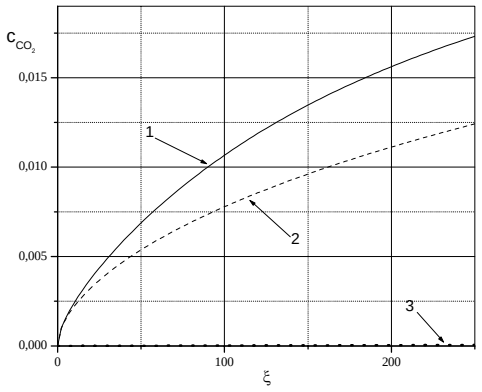

Fig. 7. Mole concentration of CO_2 lengthwise TCR

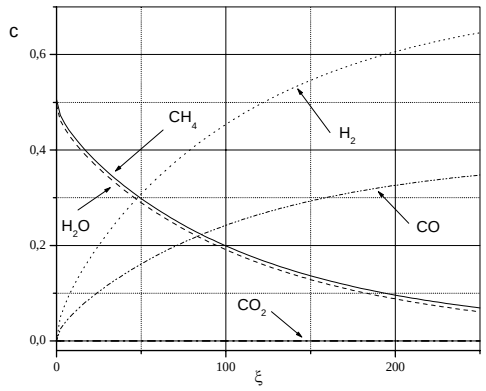

Fig. 8. General mole composition of mixture lengthwise of channel at Tw=1000C, turbulent mode

Profile characteristics

In fig. 9, 10 the profiles of temperatures T and longitudinal speed u with the channel height h are shown at ζ = 250 for catalytic wall, Tw = 700 C and two modes laminar (curve 1) and turbulent (curve 2).

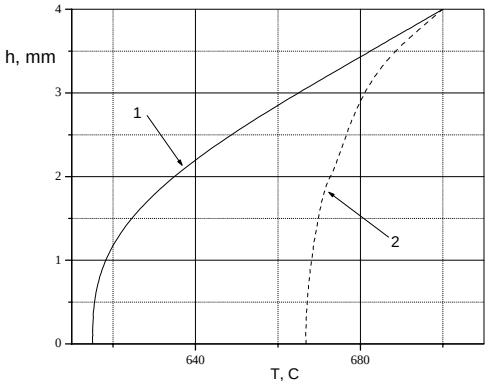

Fig. 9. Profile of temperature at ζ = 250

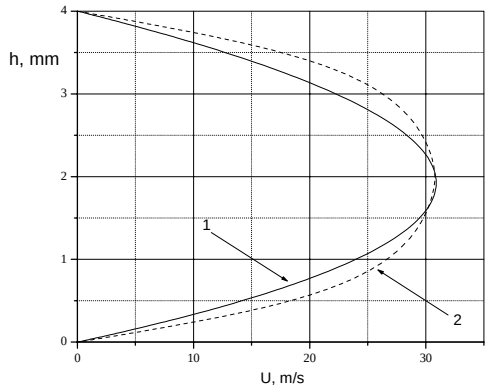

Fig. 10. Profile of a longitudinal component of speed at $\zeta = 250$

Behaviour of a temperature variation crosswise of channel (fig. 9) demonstrates that at laminar flow the mixture is heated less than at turbulent mode. Essential increasing of mixture temperature at turbulent flow in comparison to a laminar one results in decreasing of density of mixture and, therefore, at stable consumption G in increasing of longitudinal speed. However, maximum speed at turbulent flow practically does not change. The main difference in velocity profiles appears in the near-wall area. Such difference between turbulent and laminar flows causes in a turbulent flow the more intensive mixing of with the height of a channel that promotes improving TCR characteristics.

Conclusion

Flat TCR can be the effective device for cooling of heat-stressed surfaces. Generally, a turbulent flow mode in TCR is more preferable than laminar. However, it is impossible to eliminate that for cooling of extended weakly heat-stressed surfaces the laminar flow mode will be more effective than turbulent one.

In the studied flow modes the values of a specific heat flux absorbed in TCR are not significant – up to 50 - 80 kW / m^2. At the same time some tentative calculations have shown that it is possible to obtain the considerably greater specific heat fluxes removed by TCR. Therefore the multiparameter numerical studies of flat TCR are required..

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